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ABSTRACT

The invention relates to novel proteins with novel integrin and I domain activity and nucleic acids encoding these proteins. The invention further relates to the use of the novel proteins in the treatment of integrin related disorders.

Table 1. Computationally designed mutants

	WT	idolq	idolr	ido2r	jlm2r
Backbone		Ene	rgy ^b		
1ido	-1037	-1145	-1138	-1116	-678
1jlm	-1059	+82758	-840	-1000	-1086
Position			Residues		
139	I	-	-	V	_
153	M	-	-	A	-
156	F	L	W	-	-
157	V	-	-	I	-
160	V	I	-	-	-
199	V	I	I	I	-
215	I	L	L	-	V
219	V	-	-	-	I
223	F	-	-	-	L
238	V	F	F	I	I
239	V	L	L	L	-
240	I	L	L	-	-
259	A	L	L	-	-
269	I	L	-	-	-
271	V	F	-	-	-
287	I	V	V	V	-
299	V	A	I	I	-
308	I	V	-	-	-

^a Mutants are named according to the structure that was stabilized (ido or jlm), the solvation potential used (1 or 2) and the definition of core residues (q or r).

^bThe lowest energy rotamer configuration was calculated for each sequence in the 1ido structure, and cross-calculated in the 1jlm structure, using both solvent potentials; all 50 core residues were used in order to make the q and r energies comparable. Results are shown for solvent potential 1 and were similar for potential 2. A severe clash of the side-chain of F271

with the backbone caused the high energy of the 1q sequence in the 1jlm structure; no movement of the backbone is allowed by the design method.

Table 1